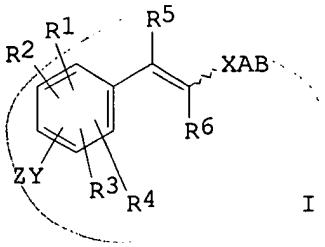
ER 64 OF 112 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:670992 CAPLUS
DOCUMENT NUMBER: 119:270992
TITLE: Heteroaryl-substituted phenylethyenyl compounds having retinoid-like biological activity
INVENTOR(S): Chandraratna, Roshantha A. S.
PATENT ASSIGNEE(S): Allergan, Inc., USA
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9316067	A1	19930819	WO 1993-US1119	19930208
W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, RO, RU, SD, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9336592	A1	19930903	AU 1993-36592	19930208
EP 626955	A1	19941207	EP 1993-905820	19930208
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07503959	T2	19950427	JP 1993-514240	19930208
JP 3499553	B2	20040223		
US 5434173	A	19950718	US 1993-126951	19930924
US 5391753	A	19950221	US 1993-126627	19930927

PRIORITY APPLN. INFO.: US 1992-833682 A 19920211
WO 1993-US1119 A 19930208
OTHER SOURCE(S): MARPAT 119:270992
GI



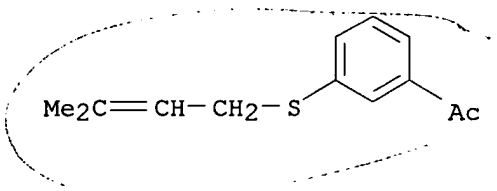
I

AB The title compds. I [A = (CH2)n, lower branched-chain C3-6 alkyl, C3-6 cycloalkyl, C2-6 alkenyl, C2-6 alkynyl; n = 0-5; B = H, (un)substituted CO2H, CH2OH, CHO, etc.; R1-R4 = H, C1-6 alkyl, halogen, C1-6 alkoxy; R5, R6 = H, C1-6 alkyl; X = divalent heteroaryl group selected from thienyl, pyridyl, furyl, pyridazinyl, pyrimidinyl, pyrazinyl, thiazolyl, oxazolyl; Y = O, S; Z = linear C1-10 alkyl, C3-10 cycloalkyl, C3-10 branched-chain alkyl, C2-10 linear alkenyl, branched-chain C3-10 alkenyl, etc.], useful as regulators of cell proliferation and differentiation, are prepared Thus, di-Et (2-carboethoxy-5-thiophenyl)methylphosphonate was condensed in the presence of NaH with 3-(3-methyl-2-thiobuten-1-yl)benzaldehyde, producing 5-[E-2-[3-(3-methyl-2-thiobuten-1-yl)phenyl]ethenyl]-2-thiophenecarboxylate (II). II demonstrated 80% inhibitory concentration of 12-O-tetradecanoyl-phorbol-13-acetate-induced ornithine decarboxylase activity of 147 nM.

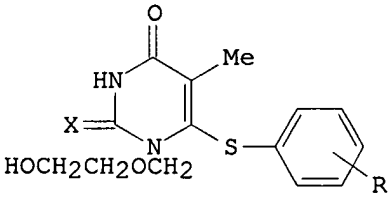
IT **151330-70-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of heteroaryl-substituted phenylethenyl compds. having retenoid-like activity)

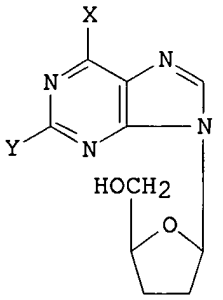
RN 151330-70-0 CAPLUS
CN Ethanone, 1-[3-[(3-methyl-2-butenyl)thio]phenyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 65 OF 112 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:530919 CAPLUS
DOCUMENT NUMBER: 119:130919
TITLE: QSAR of HIV inhibitors
AUTHOR(S): Hansch, Corwin; Zhang, Litai
CORPORATE SOURCE: Dep. Chem., Pomona Coll., Claremont, CA, 91711, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1992), 2(9), 1165-9
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB Quant. structure-activity relationships (QSAR) are derived for two sets of HIV inhibitors: 1-[2-hydroxyethoxy)methyl]-6-(X-phenylthio)thymines and thiothymines (I, R = e.g., 2- or 3-Me, 3-halo, 2- or 3-OMe, X = O or S) and dideoxypurine ribofuranosides (II, X = e.g., chloro or NH2, Y = halo, SH, or NH2). The hydrophobic and especially the steric properties of substituents determine relative potencies of the derivs.

IT **137897-75-7**
RL: BIOL (Biological study)
(HIV virus inhibitor, QSAR of)

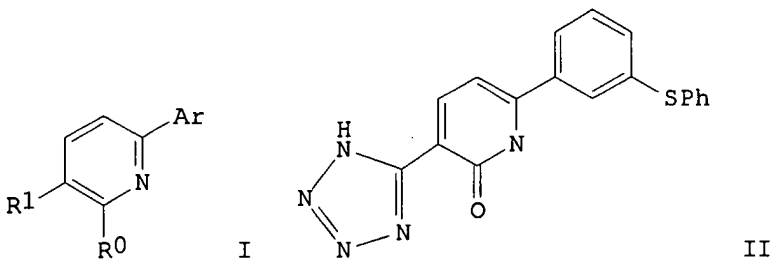
RN 137897-75-7 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 6-[(3-acetylphenyl)thio]-1-[(2-hydroxyethoxy)methyl]-5-methyl- (9CI) (CA INDEX NAME)

F 112 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:490296 CAPLUS
DOCUMENT NUMBER: 117:90296
TITLE: Preparation of 6-phenyl-3-(5-tetrazolyl)pyridin-2(H)-one derivatives as cyclic AMP-dependent protein kinase agonists
INVENTOR(S): Porter, Roderick Alan; Murray, Kenneth John; Warrington, Brian Herbert; Prain, Hunter Douglas
PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK
SOURCE: PCT Int. Appl., 78 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9206085	A1	19920416	WO 1991-GB1663	19910926
W: AU, CA, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
CA 2091989	AA	19920329	CA 1991-2091989	19910926
AU 9185431	A1	19920428	AU 1991-85431	19910926
AU 644016	B2	19931202		
ZA 9107697	A	19930428	ZA 1991-7697	19910926
EP 550576	A1	19930714	EP 1991-917244	19910926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06501254	T2	19940210	JP 1991-515556	19910926

PRIORITY APPLN. INFO.: GB 1990-21184 19900928
GB 1991-17657 19910815
WO 1991-GB1663 19910926

OTHER SOURCE(S): MARPAT 117:90296
GI



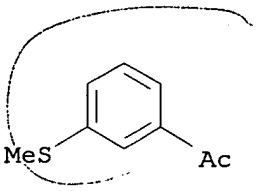
I II

AB The title compds. [I; R0 = HO or its precursor; R1 = tetrazolyl or its precursor; Ar = Ph optionally substituted by C1-6 alkyl(thio), C2-6 alkenyl, C1-6 alkoxy, C1-6 polyfluoroalkyl, C3-6 cycloalkyl, phenyl(thio), halo, NR2, etc.; R = H, C1-6 alkyl, X(CH2)nY attached to the adjacent C atoms of the Ph ring; X, Y = CH2, O; n = 1-3; with a proviso] or their pharmaceutically acceptable salts, having antiproliferative, antiaggregatory, muscle-relaxing, lusitropic, etc., activities, were prepared Condensation reaction of 2.05 g 3-PhSC6H4COMe with 1.19 g Me2NCH(OMe)2 in DMF gave 1.72 g 3-PhSC6H4COCH:CHNMe2 which was refluxed for 1 h in DMF with 0.76 g NaOMe and 0.59 g H2NCOCH2CN to give 1.09 g 3-cyano-6-(3-phenylthiophenyl)pyridin-2(1H)-one. Cyclocondensation of the latter (0.79 g) with NaN3 in N-methylpyrrolidin-2-one at reflux gave 0.77 g title compound II. The latter in vitro inhibited (IC50 values in

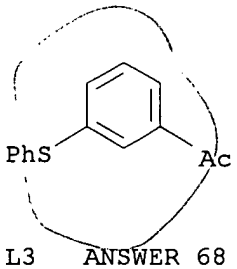
parentheses) proliferation of human colorectal cells SW-620 (56-90 μM), NRK-52 (46-48 μM), and HT-29 (55-66 μM). II in vitro inhibited spontaneously developed tension of guinea pig trachea strips with IC50 = 6.5 μM, and at 30-100 μM in vitro caused a 10-20% decrease of the rabbit cardiac muscle relaxation time. Approx. 58 I were prepared and 57 I are claimed.

IT **1441-99-2**, 3'-Methylthioacetophenone **26388-18-1**, 3'-(Phenylthio)acetophenone
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of protein kinase agonists)

RN 1441-99-2 CAPLUS
CN Ethanone, 1-[3-(methylthio)phenyl]- (9CI) (CA INDEX NAME)



RN 26388-18-1 CAPLUS
CN Ethanone, 1-[3-(phenylthio)phenyl]- (9CI) (CA INDEX NAME)

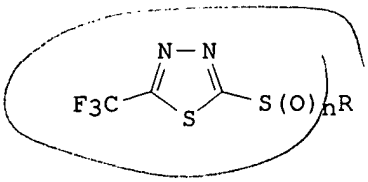


L3 ANSWER 68 OF 112 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:59876 CAPLUS
DOCUMENT NUMBER: 116:59876
TITLE: Structure-activity relationships of 1-[(2-hydroxyethoxy)methyl]-6-(phenylthio)thymine analogs: effect of substitutions at the C-6 phenyl ring and at the C-5 position on anti-HIV-1 activity
AUTHOR(S): Tanaka, Hiromichi; Takashima, Hideaki; Ubasawa, Masaru; Sekiya, Kouichi; Nitta, Issei; Baba, Masanori; Shigeta, Shiro; Walker, Richard T.; De Clercq, Erik; Miyasaka, Tadashi
CORPORATE SOURCE: Sch. Pharm. Sci., Showa Univ., Shinagawa, 142, Japan
SOURCE: Journal of Medicinal Chemistry (1992), 35(2), 337-45
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

ANSWER 87 OF 112 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:547051 CAPLUS
DOCUMENT NUMBER: 87:147051
TITLE: 2-Substituted 5-trifluoromethyl-1,3,4-thiadiazoles as fungicides and insecticides
INVENTOR(S): Reisdorff, Josef Helmut; Brandes, Wilhelm; Scheinpflug, Hans; Homeyer, Bernhard; Roessler, Peter
PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 68 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2533604	A1	19770210	DE 1975-2533604	19750726
CS 193555	P	19791031	CS 1976-4542	19760708
RO 69553	P	19800815	RO 1976-86934	19760710
SE 7608361	A	19770127	SE 1976-8361	19760722
AU 502962	B2	19790816	AU 1976-16140	19760722
SU 849976	A3	19810723	SU 1976-2385098	19760722
BE 844442	A1	19770124	BE 1976-169166	19760723
DK 7603330	A	19770127	DK 1976-3330	19760723
ES 450091	A1	19770716	ES 1976-450091	19760723
BR 7604791	A	19770802	BR 1976-4791	19760723
DD 127533	C	19770928	DD 1976-194037	19760723
CA 1072965	A1	19800304	CA 1976-257696	19760723
JP 52014768	A2	19770203	JP 1976-87760	19760724
NL 7608273	A	19770128	NL 1976-8273	19760726
FR 2319635	A1	19770225	FR 1976-22732	19760726
FR 2319635	B1	19800509		
AT 348292	B	19790212	AT 1976-5475	19760726

PRIORITY APPLN. INFO.: DE 1975-2533604 19750726
GI

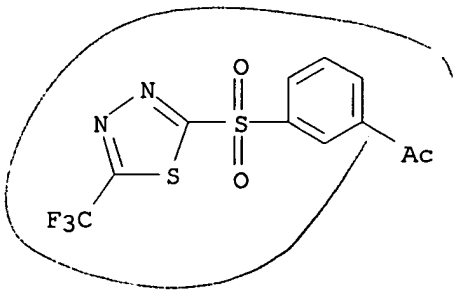


I

AB The title compds. I (R = substituted alkyl, substituted aryl, heterocycle with 1-4 heteroatoms, substituted benzimidazole, etc.; n = 0-2) are fungicides and insecticides. Thus, in greenhouse expts. a composition containing 0.00062% 2-(3,4-dichlorophenylsulfonyl)-5-(trifluoromethyl)-1,3,4-thiadiazole gave 100% protection to apple seedlings from apple scab (Fusicaldium dendriticum). No survivors resulted in tests with Tenebrio molitor larvae on soil treated with 10 ppm of the above compound

IT **62617-24-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

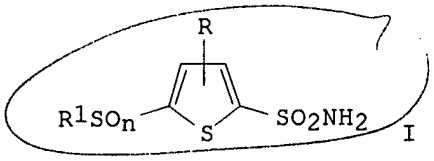
RN 62617-24-7 CAPLUS
CN Ethanone, 1-[3-[[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)


O
N
N
S
S
O
Ac
F3C

ER 88 OF 112 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:405796 CAPLUS
DOCUMENT NUMBER: 87:5796
TITLE: Thiophene-2-sulfonamide derivatives and their use as therapeutic agents
INVENTOR(S): Barnish, Ian T.; Cross, Peter E.; Dickinson, Roger P.
PATENT ASSIGNEE(S): Pfizer Ltd., UK
SOURCE: Brit., 27 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1459571	A	19761222	GB 1974-39753	19750910

PRIORITY APPLN. INFO.: GB 1974-39753 19750910
GI

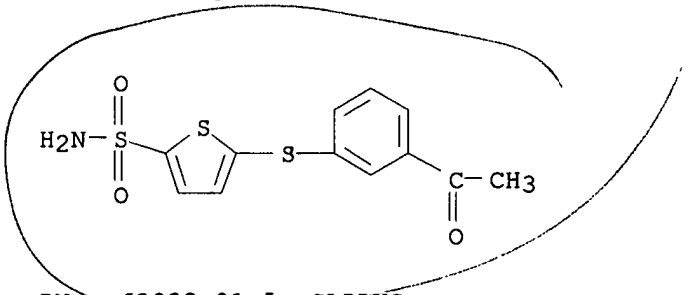


I

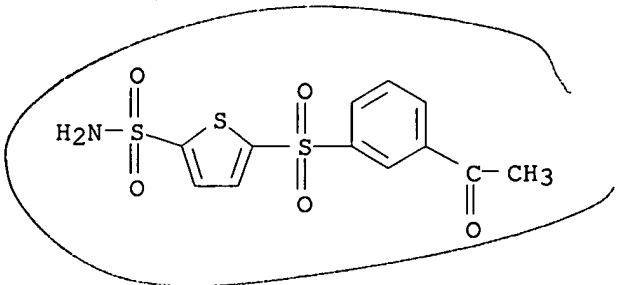
AB About 200 title compds. I (R = H, halo, Me, NO2, MeO; R1 = carbocyclic or heterocyclic aromatic group; n = 0, 1, 2), useful as cerebral vasodilators (no data), were prepared Most I (n = 0) were prepared from R1SH by condensation with 5-halothiophene-2-sulfonamides, from R1Br by condensation with 2-mercaptothiophenes, or from 2-(arylthio)thiophenes by successive sulfonation, conversion to the sulfonyl chloride, and treatment with NH3. Most I (n = 1,2) were prepd,. from I (n = 0) by oxidation Some I also show anticonvulsant activity (no data).

IT **63032-02-0P 63032-81-5P 63033-42-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(cerebral vasodilator, preparation of)

RN 63032-02-0 CAPLUS
CN 2-Thiophenesulfonamide, 5-[(3-acetylphenyl)thio]- (9CI) (CA INDEX NAME)



RN 63032-81-5 CAPLUS
CN 2-Thiophenesulfonamide, 5-[(3-acetylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 63033-42-1 CAPLUS
CN 2-Thiophenesulfonamide, 5-[(3-acetylphenyl)sulfinyl]- (9CI) (CA INDEX NAME)